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The study of high-frequency dynamics in liquid magnesium by memory-function formalism and computer simulation molecular dynamics

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Abstract

The study of structure and dynamics of particles in liquid magnesium at the two thermodynamical states (at the temperature T = 953 K and T = 1063 K) has been performed by computer simulation molecular dynamics with the "glue" interparticle potential. The calculated equilibrium terms are compared with the experimental data on X-ray scattering. The results of comparative analysis to show adequacy of choice of the interparticle potential for liquid magnesium. The study of collective properties of the magnesium particles on the basis of the dynamic structure factor, S(k,W), for eight wave-numbers k = 0.5, 0.7, 0.9, 1.1, 1.4, 1.6, 1.8 H 2.0 A-1 are carry out. The theoretical analysis of S(k,W) by Zwanzig-Mori's memory-function formalism on the basis of N.N. Bogoliubov's ideas about reduced description of statistical systems and the hierarchy of relaxation time-scales are executed. The results of theoretical calculations are in a good agreement with computer simulation molecular dynamics data.

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